QUALITY ASSURANCE PROJECT PLAN AND PROJECT WORK PLAN

SIMULATED FATE AND TRANSPORT OF ETHYLENE DIBROMIDE IN THE SANTE FE AQUIFER NEAR KIRTLAND AIR FORCE BASE, ALBUQUERQUE, NEW MEXICO

U.S. EPA
REGION 6
MULTIMEDIA PLANNING AND PERMITTING DIVISION

United States Environmental Protection Agency

Prepared by:
Scott Ellinger, P.G.
Mail Code 6PD-C
214-665-8408

February 23, 2012

GROUP A PROJECT MANAGEMENT
A1 TITLE AND APPROVAL SHEET

TITLE:

SIMULATED FATE AND TRANSPORT OF ETHYLENE DIBROMIDE IN THE SANTE FE AQUIFER NEAR KIRTLAND AIR FORCE BASE, ALBUQUERQUE, NEW MEXICO

PREPARED BY:

Name: Scott Ellinger, P.G.
Title: Geologist, Corrective Action/Waste Minimization Section

Signature: ________________________________ Date: ____________

PEER REVIEWED BY:

Name:
Title:

Signature: ________________________________ Date: ____________

APPROVED BY (EPA):

Name: Ben Banipal, P.E.
Title: Chief, Corrective Action/Waste Minimization Section

Signature: ________________________________ Date: ____________

A2 TABLE OF CONTENTS

A 2.1 LIST OF FIGURES

A.2.2 LIST OF TABLES

A.2.3 LIST OF EQUATIONS

A3 DISTRIBUTION LIST

After final approval of this QA Project Plan and Project Work Plan, the Project Manager will transmit copies to the individuals and organizations below.

U.S. Environmental Protection Agency, Region 6

- Donald Johnson
  Regional Quality Assurance Manager
  Management Division (6MD)

- Charles Ritchey
  Division Quality Assurance Officer
  Multimedia Planning and Permitting Division (6PD)

New Mexico Environment Department

- William Moats
  Staff Manager, Albuquerque Group
  Hazardous Waste Bureau
  New Mexico Environment Department
  5500 San Antonio, NE
  Albuquerque, NM 87109

  Phone: 505-222-9551
  Email: William.Moats@state.nm.us

- John E. Kieling
  Acting Chief
  Hazardous Waste Bureau
  2905 Rodeo Park Drive East, Building 1
  Sante Fe, New Mexico 87508-6303

  Phone: 505-476-6035
  Email: John.Kieling@state.nm.us

A4 PROJECT AND TASK ORGANIZATION

All environmental monitoring and measurement efforts mandated or supported by the U.S. Environmental Protection Agency (EPA) are subject to a centrally managed quality assurance (QA) system. The EPA Quality System defined in EPA Order 5360.1 A2, *Policy and Program Requirements for the Mandatory Agency-wide Quality Syste*m, includes coverage of environmental data produced from models. Environmental data includes any measurement or information that describe environmental processes, locations, or conditions; ecological or health effects and consequences; or the performance of environmental technology. For EPA, environmental data includes information collected directly from measurements, produced from models, and compiled from other sources such as databases or literature. The EPA Quality System is based on an American National Standard, ANSI/ASQC E4-1994.

Consistent with the National Standard, E4-1994, Section §6.a.(7) of EPA Order 5360.1 A2 states that EPA organizations will develop a Quality System that includes approved Quality Assurance Project Plans (QAPP), or equivalent documents defined by the Quality Management Plan, for all applicable projects and tasks involving environmental data with review and approval having been made by the EPA QA Manager (or authorized representative defined in the Quality Management Plan). More information on EPA's policies for QA Project Plans is provided in Chapter 5 of U.S. EPA (2000), *EPA Quality Manual for Environmental Programs*. This guidance helps to implement the policies for models defined in Order 5360.1 A2.

Any party that generates data under the QA program is responsible for implementing minimum procedures to ensure that the precision, accuracy, completeness, sensitivity, comparability, and representativeness of its data are known and documented. Each party must prepare a QAPP for each environmental data collection effort. In response to this requirement, the EPA Project Manager has prepared this QAPP which presents the overall project description, project organization and responsibilities, and QA objectives associated with the ground-water modeling to be conducted. This project-specific QAPP complies with all relevant elements of U.S. EPA (2002), *EPA Guidance for Quality Assurance Project Plans for Modeling,* and has undergone peer-review.

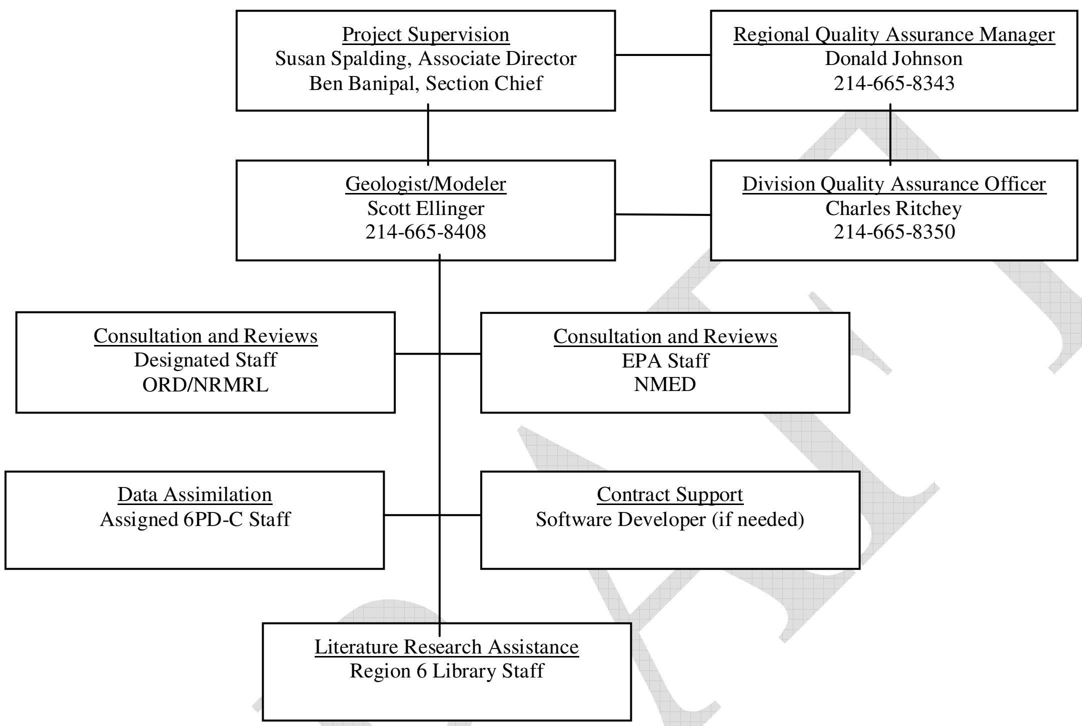
To complete this modeling project, the EPA Region 6 Multimedia Planning and Permitting Division (6PD) will develop a ground-water model for a portion of the Sante Fe aquifer in the vicinity of Kirtland Air Force Base (KAFB) in Albuquerque, N.M., and nearby drinking water supply wells. Simulating subsurface phenomena, such as ground-water flow and contaminant fate and transport, is a complex process involving development of a conceptual model of the system, selection of a model code that is capable of performing the simulation, transforming aspects of the conceptual model into their mathematical counterparts, developing numerical output, and evaluating model results. To facilitate major aspects of model development, 6PD will seek input from several organizations including the New Mexico Environment Department, the EPA National Risk Management Research Laboratory (NRMRL) Robert S. Kerr Environmental Research Center in Ada, Oklahoma, and may consult software development companies for data processing assistance if needed.

Overall project supervision lies with the Management of 6PD. 6PD management provides direction to technical staff which is responsible for overall model development. The Region 6 Quality Assurance Manager and Division Quality Assurance Officer provide guidance and support during QAPP development and processes for model peer reviews to ensure that the Agency's Quality Assurance requirements are being met. The EPA NRMRL will be requested to assist by providing advice on model set up, model calibration, sensitivity analysis, interpreting modeling results, and other related modeling activities. EPA will collaborate with NMED by seeking NMED's input during the model development process, and NMED will review model output and related documentation to determine whether modeling goals have been achieved. Additional EPA staff, as assigned, will assist by providing literature research and reviews to gather supporting data and perform data synthesis. The EPA Region 6 Library will assist by conducting literature searches and by ordering and obtaining critical information and data.

The overall purpose of this modeling study is to evaluate the fate and transport of Ethylene Dibromide (EDB) in groundwater within the Sante Fe aquifer near Kirtland Air Force Base. If sufficient data are not available to support the development of a contaminant fate and transport model for the specified project goals, and/or if data are not sufficient for a related groundwater flow model, then documentation will be prepared to outline the types of data needed before model development can proceed. In the event that only ground-water flow modeling is possible, then only the relevant sections of this QAPP will be in effect and considered as part of the modeling effort.

The reader is referred to the Project Geologist/Modeler for any questions or concerns related to this combined QAPP and General Work Plan. The official, approved QAPP and General Work Plan will be maintained by the Project Geologist/Modeler in the Mulitmedia Planning and Permitting Division. During the course of this project certain conditions, processes, and procedures inherent to modeling may change. If such changes cause any significant changes to the QAPP, the Region 6 Quality Assurance Manager and/or Division Quality Assurance Officer will be notified.

Project Organization



A5 DEFINITION AND BACKGROUND OF PROBLEM

In 1999, a leak of jet fuel, jet propellant 8 (JP-8), was discovered from underground pipelines at the KAFB Bulk Fuels Facility. Oversight of the investigation and cleanup was originally overseen by the NMED Ground Water Quality Bureau under the Compliance and Enforcement Program which administers the New Mexico Water Quality Control Commission regulations – the fuel leak was originally viewed as a product release rather than an issue of hazardous waste. In April 2010, oversight of the fuel spill was transferred to the NMED Hazardous Waste Bureau for RCRA Corrective Action under KAFB's hazardous waste permit. Upon further investigation of soil and groundwater contamination, the spill was found to also include JP-4 and aviation gas. Aviation gas had been used in the fuel system prior to 1980; therefore, the leak occurred prior to 1980. Fuels have percolated down to the drinking water aquifer, approximately 500 feet deep. The EDB plume extends the farthest, approximately 6,000 feet in length, but has not been fully delineated. NMED has estimated the volume of fuel released to be 8 million gallons.

Approximately 3,200 feet downgradient of the EDB plume known extent is KAFB water supply well, KAFB-3, and approximately 5,200 feet downgradient is Albuquerque Bernalillo County Water Utility Authority (ABCWUA) water supply well, Ridgecrest No. 5. Ridgecrest No. 5 is one of five water supply wells in the Ridgecrest well field. Still other ABCWUA wells, wells of the Burton well field, are situated just northwest of the known EDB plume. Groundwater modeling of the fuel plume is needed to determine the fate and transport of EDB in groundwater from the source at the BFF to the nearest water supply wells and also to model the capture zone of the proposed groundwater pump and treat system. Figure 1 is a site location map of the area of the area of interest showing the current location of the EDB in relation to nearby water supply wells.

With groundwater modeling assistance from EPA, NMED is hoping to gain a better understanding of the fate and transport of EDB in the Sante Fe aquifer between the KAFB Bulk Fuels Facility and the KAFB and ABCWUA water supply wells.

<u>Specific Technical Goals</u>

As with any groundwater modeling project, specific goals are required in order to develop an appropriate model setup to produce the desired output. The two modeling goals below were specified by NMED.

1. Model the fate and transport of EDB in groundwater at the KAFB Bulk Fuels Facility, by starting with the current highest concentrations of EDB in groundwater beneath the

source and predict the concentrations of EDB that would be expected to reach the production wells if nothing was done to mitigate the problem.

2. Model the capture zone of two proposed extraction wells referred to as the Light Non-Aqueous Phase Liquid (LNAPL) Containment System.

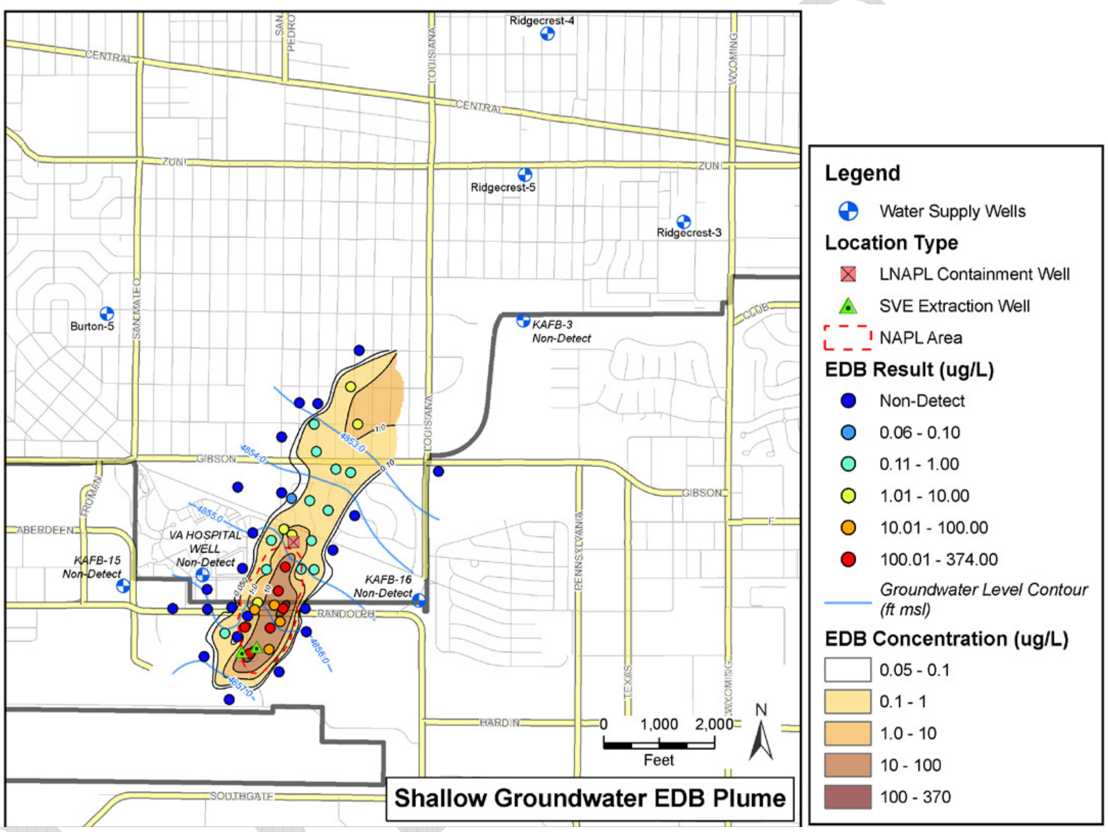


Figure 1: Map showing approximate plume extent and water supply wells.
Map source: KAFB December 2011 public meeting slides.

A6 PROJECT/TASK DESCRIPTION AND SCHEDULE

6PD will perform modeling related activities in accordance with standard accepted scientific and modeling practices and guidelines as referenced below. EPA will utilize applicable sections from a number of modeling guidance documents and manuals to ensure that modeling procedures are being properly conducted. These documents will include the U.S. EPA Guidance for Quality Assurance Project Plans for Modeling (EPA 2002), the U.S. EPA Office of Solid Waste and Emergency Response Groundwater Model Compendium (1994) , U.S. Army

Corps of Engineers (1999) engineering and design manual, and various software manuals specific to the pre and post data processor. Further, EPA will refer to applicable sections of guidelines published by the American Society for Testing and Materials (ASTM) which publishes consensus standards for a variety of fields, including ground-water modeling. The ASTM Subcommittee D18.21 on ground-water and vadose zone investigations has standard guides related to ground-water modeling including the following publications.

- ASTM D-5447: Application of a Groundwater Flow Model to a Site-Specific Problem
- ASTM D-5718: Documenting a Ground-Water Flow Model Application
- ASTM D-5609: Defining Boundary Conditions in Ground-Water Modeling
- ASTM D-5610: Defining Initial Conditions in Ground-Water Modeling
- ASTM D-5611: Conducting a Sensitivity Analysis for a Ground-Water Flow Model Application
- ASTM D-5490: Comparing Ground-Water Flow Model Simulations to Site Specific Information
- Additional (non-ASTM): US Geological Survey: Guidelines for Evaluating Groundwater Flow Models, 2004-5038.

EPA will also refer to other published information, when needed, such as professional scientific journals and articles identified from a search of pertinent literature in addition to the above sources of information.

The development and completion of a ground-water model ideally would follow several basic steps to achieve an acceptable representation of the hydrogeologic system and to document modeling results for the end-user, decision-maker, or regulator. These steps include:

- Identify and define modeling goals, objectives, and uses
- Develop project work plan
- Develop Quality Assurance Project Plan
- Collect, organize, and interpret data
- Prepare a conceptual model
- Set up numerical model
- Calibrate model
- Run model for flow simulation
- Run model for fate and transport (data permitting)
- Perform post-simulation analysis
- Validate model
- Evaluate overall modeling effectiveness
- Determine whether goals and objectives have been/are being met

- Determine preliminary results and level of accuracy and error
- Reiterate modeling steps as needed
- Final results and report

There are many existing published and unpublished reports describing the geology and hydrogeology of the Albuquerque Basin and the Kirtland area including groundwater modeling studies. The conceptual model for this project will utilize existing information as necessary and will include any original pre-modeling data analyses as required to determine model design. The conceptual model may be included as a separate section in the final modeling report.

The final modeling report for this project will include a thorough description of model setup, model calibration, predictive simulations, sensitivity analysis, uncertainties, and conclusions. The following list is representative of the content headings of many modeling reports.

- Title page
- List of tables
- List of figures
- Abstract
- Introduction
- Model goals
- Hydrogeologic characterization
- Conceptual model
- Codes used
- Input parameters and model framework
- Model calibration
- Sensitivity analysis
- Simulations performed, interpretations
- Uncertainties
- Conclusions and recommendations
- References
- Tables
- Figures
- Well data

Establish Modeling Goals	Nov./11
Literature Search	Nov./11
Information Review	Ongoing
Develop Combined Workplan/QA Plan (draft)	Feb./12
Develop preliminary computer model framework	Feb.-Mar./12
Conceptual model development	Mar./12
Develop computer input files	Mar.-Apr./12
Site Visit	April 12
Review of conceptual model (meeting or conference call)	April 12
Meeting at Kerr Research Laboratory (review model setup)	May 12
Groundwater flow and EDB model calibration	May-June/12
Model execution assessment (review by software company)/revisions	June/12
Meeting with NMED on model output	June/12
Begin report preparation	July/12

Table 1: Project Schedule
(Schedule is approximate and contingent upon fulfilling data quality requirements. Schedule will be modified or extended as necessary to reflect additional data needs and time requirements.)

A7 QUALITY OBJECTIVES AND CRITERIA FOR MODEL INPUT AND OUTPUT

A.7.1 MODEL DEVELOPMENT AND QUALITY REVIEW CRITERIA

The EPA data quality objective (DQO) process is a systematic planning tool designed to ensure that the measurement data collected are of the type, quantity, and quality that are the most appropriate for supporting the decisions that will be based on these data (EPA 1999a; 1999b). Data quality depends on the intended use of the data and decisions. For projects that require data collection or environmental data produced from models, EPA's DQO process will be followed. Environmental data includes any measurement or information that describe environmental processes, location, or conditions; ecological or health effects and consequences; or the performance of environmental technology. For EPA, environmental data includes information collected directly from measurements, analysis produced from models, and compiled from other sources such as databases or literature.

EPA has specified use of the Graded Approach in allowing the application of quality assurance and quality control activities to be adapted to meet the rigor of the need by the project at hand. The Graded Approach is a scale indicating the level of QA needed relative to two main aspects of modeling project: (i) the intended use of the model and, (ii) project scope and magnitude. NMED has specified the intended use of the Sante Fe aquifer EDB fate and transport model as follows:

- Confirm the results of KAFB's model, and thus, will be used to assess whether the recommended final remedy would be expected to be successful in cleaning the groundwater up and how much time would be required to stabilize the contaminant plumes and complete final clean up.

- The model will also be used to predict if and when the EDB contaminant plume would reach water supply wells at a concentration exceeding the water quality standard of 0.050 ug/L. The model and its results will be made available for public inspection. There is no current or anticipated litigation concerning this project.

Utilizing a level of model data quality commensurate with the intended use of the model will be integral to the modeling process. The intention is to utilize sufficient data quality to produce model output where simulated groundwater flow closely matches field observations (calibration), and produces reliable results for predicted future EDB fate and transport in the Sante Fe aquifer. Therefore, based on the purpose for obtaining model generated information, and on discussions with NMED, two DQOs for this project have been determined:

- Utilize reliable data enabling Modflow, Modpath, and MT3D (or alternative) model codes to be employed to simulate/determine ground-water flow directions and EDB contaminant fate and transport, with reasonable match to field measurements, in the Sante Fe aquifer in and around the KAFB bulk fuels facility and nearby water supply wells.

- Utilize reliable data to evaluate the effects of pumping on groundwater flow and EDB contaminant transport related to capture zones created by proposed extraction wells.

To meet the DQO’s stated above, systematic modeling guidelines for meeting data quality will be followed when acquiring, generating, and handling data to develop the flow and transport model. These guidelines include agency guidance and ASTM guides previously mentioned, and an EPA Office of Air and Radiation (OAR) model checklist to ensure model completeness and proper execution (EPA 1996). The OAR guidance describes the activities and thought process that should be a part of a model application, documentation, and review of ground-water modeling. Not all elements of the guidance are strictly applicable to this modeling project. The guidance is divided into a series of elements which are typical of most modeling studies. These elements are listed below.

- Modeling Application Objectives (Section A.7.1.a)
- Conceptual Model (Section A.7.1.b)
- Figures and Tables (Section A.7.1.c)
- Review Considerations for Conceptual Model Formulation (Section A.7.1.d)
- Model (code) Selection (Section A.7.1.e)
- Model Construction and Calibration (Section A.7.1.f)
- Sensitivity/Uncertainty Analysis (Section A.7.1.g)

A.7.1.a. MODELING OBJECTIVES AND DATA REQUIREMENTS

The objectives of a modeling study should be clearly specified as early as possible. (Objectives in this context means overriding project goals and intermediate task objectives). All assumptions incorporated within the modeling objectives should be reviewed with respect to reality and their potential impacts on project objectives. The level of model complexity and, in turn, the type of model required (e.g., numerical or analytical) should be documented as part of the modeling objectives.

The definition of modeling objectives is important. It is necessary to give reviewers a clear understanding about what the model results will be used for and how these results fit into the development of the model.

- The purpose and scope of the model should be clearly indicated.

- In the summary and conclusions of the final report, each objective should be discussed separately in context of how the modeling was used to meet the objective and the degree to which the objective was met.

- The data required to construct a conceptual model should be described and the relevance of the data to ground-water flow and fate and transport should be discussed.

- The source of data should be presented. Discuss which data will be or was collected in the field, versus taken from the literature and/or model calibration.

- The uncertainties associated with data should be discussed. Discuss field collection methods if possible and reliability of literature values. A probable range in which the parameters will fall should be assigned prior to the modeling analysis.

- The general sensitivity of data to the determination of ground-water flow and fate and transport should be discussed.

- Limitations and weaknesses in data should be presented, as well as plans to enhance data.

- Recommendations should be presented detailing additional data needed to increase confidence in the modeling results.

A.7.1.b. CONCEPTUAL MODEL DEVELOPMENT

Prior to documenting the type of model used and how it was constructed, the report should contain a thorough discussion of the conceptual model that is the foundation of the mathematical model. The conceptual model does not necessarily need to restate all of the information known about the region being modeled. Rather, the conceptual model should be described in terms of the assumptions made to simplify the system. The conceptual model should also list data gaps and their impact on the modeling results. Typical information that should be provided with respect to the conceptual model includes the following:

- The hydrogeologic system should be described in detail including lithologic contacts, facies changes, discrete features, and spatial variations of geologic units and their hydraulic properties. The rationale for the variability of the properties should be explained (e.g., depositional history).

- The boundaries of the system should be described in a water budget analysis (evapotranspiration, runoff, pumping and recharge rates). The methodology for determining individual components of the water budget should also be included.

- The geometry of the system should be presented in three dimensions with a rationale for possible simplification. For example, the analysis of the unsaturated zone may be reduced to two dimensions.

- The rationale for any simplifications (e.g., steady state) made to the conceptual model should be presented.

- Uncertainties in the conceptual model should be presented and related to earlier discussions of data limitations and uncertainties.

- The contaminant source term should be described.

A.7.1.c. FIGURES AND TABLES

The following list is meant to show the types of figures and tables that may be included to describe the conceptual model. Although some may not necessarily be required or available for every site, appropriate figures and tables should be used to supplement written descriptions. Some may be included as attachments or by reference.

- Map showing location of study area.
- Maps and cross sections showing the thickness of the unsaturated zone.
- Geologic map and cross sections indicating the areal and vertical extent of the local or regional system.
- Topographic map indicating surface water bodies.
- Contour maps showing the tops and/or bottoms of the aquifers and confining units.
- Isopach maps of hydrostratigraphic units.
- Maps showing extent and thicknesses of stream and lake sediments.
- Maps indicating any discrete features.
- Maps and cross sections showing the unsaturated zone properties.
- Potentiometric surface maps of aquifer(s) showing hydraulic boundaries.
- Maps, cross sections, or tables showing storage properties of the aquifers and confining units.
- Maps, cross sections, or tables showing hydraulic conductivity of the aquifers, confining units, and stream and lake sediments.
- Maps, hydrographs, and/or tables of water-budget information, including evapotranspiration, runoff, ground-water recharge, ground-water pumping, and gains/losses between ground-water and surface water.

- Maps, cross sections, or tables indicating effective porosity of the aquifers (required for particle tracking).
- Maps and cross-sections indicating transport parameters.
- Areal and cross-sectional isoconcentration maps of contaminants.
- Time-series graphs of contaminant concentrations.
- Relevant source term information.

A.7.1.d. REVIEW CONSIDERATIONS FOR CONCEPTUAL MODEL FORMULATION

- Is the conceptual model consistent with field data?
- Are conceptual model simplifications justified?
- Are sufficient data available to meet the modeling objectives?
- Have database deficiencies been clearly identified and modeling implications discussed?
- Have the natural boundaries of the aquifer system been described?

A.7.1.e. MODEL (CODE) SELECTION

The selected computer program(s) (code) should be described with regard to its flow, contaminant transport and transformation processes, mathematics, hydrogeologic system representation, boundary conditions, and input parameters. The reliability of the code should be assessed including a review and listing of the following information. Mainstream groundwater modeling programs such as Modflow are well documented codes and are described in Section B 10.

- Peer reviews of the model's theory (e.g., a formal review process by an individual or organization acknowledged for their expertise in ground-water modeling or the publication of the theory in a peer reviewed journal).

- Verification studies (e.g., evaluation of the model results against laboratory tests, analytical solutions, or other well accepted models being able to address PCE/TCE degradation).

- Relevant field tests (i.e., the application and evaluation of the model to site-specific conditions for which extensive data sets are available).

- Code acceptability in the user community as evidenced by the quantity and type of use.

- Full model documentation.

- Publication and peer review of model code testing.

The assumptions in the model code should be analyzed with regard to their impact upon the modeling objectives and site-specific conditions. Any and all discrepancies between the modeling requirements (i.e., as indicated by study objectives, conceptual model, and available data) and the capabilities of the selected model should be identified and justified. For example, the implications of the selected code supporting 1, 2, or 3-dimensional modeling, providing steady state versus transient modeling, or requiring simplifications of the conceptual model should be discussed. Other criteria that should be documented include:

- Selection criteria should be clearly presented for the selected code(s).

- The general features of the code should be discussed, including whether the code is a proprietary version of the code used for modeling, solution methodologies for the flow and transport equations, hardware requirements, degree of code testing, and availability of source code and documentation.

- The assumptions and limitations should be described, particularly those pertaining to the conceptual model. These would include code dimensionality, ability to simulate heterogeneities, and flow and transport through the unsaturated zone.

- The basis for regulatory acceptance should be discussed which may include a history of use, particularly for applications in a similar regulatory context.

- Documentation on the source code should be available, with an executable version of the code and data sets relevant to the problem.

A.7.1.f. MODEL CONSTRUCTION AND CALIBRATION

Model construction includes the design of the model grid for numerical models, selection and positioning of boundary conditions, and definition of hydraulic and chemical properties. The model report should document the assumptions and reasons that form the basis of model construction.

For numerical models, generally acceptable rules of grid design and time step selection should be applied to meet the modeling objectives. The grid chosen for each modeling study should be justified and, if possible, grid convergence analyses should be documented.

When a numerical model is used the mapping of the location of the boundary conditions and other geometric details (e.g., wells, repository, and contaminant sources) on the grid should be evaluated. If arbitrary or artificial boundaries are used, justification for their use should be given and evidence presented to demonstrate that their use does not adversely impact the model results within the area of interest.

The input estimation process whereby data are converted into model inputs (e.g., spatial and temporal interpolation, extrapolation or Kriging, or averaging) should be described. This description should include a map or table containing the spatial location and the associated values of data used to perform the interpolation. Important considerations include:

Layering and Gridding

- The grid should be presented as an overlay of a map of the area to be modeled.
- The rationale for the selection of the grid spacing, number of model layers, and the resulting number of nodes and elements should be given.
- The grid should be refined as needed to properly define boundary conditions such as rivers and locations where the aquifer is stressed.
- A vertical cross section of the modeled area which displays the vertical layering of the model with respect to its hydrogeology should be included.
- Horizontal and vertical grid coordinates and elevations should be identified clearly.

Boundary and Initial Conditions

- The report should clearly identify assigned boundaries and initial conditions in figures and tables.
- Selection of all boundaries and initial conditions should be justified.
- Uncertainty surrounding boundaries and initial conditions should be discussed.

- The boundaries should be positioned to ensure that simulations will not be adversely affected by pumping wells or other features that stress the system.

- Flow boundaries should coincide with natural features and/or hydraulic controls (e.g., ground-water divides).

- The areal recharge should not exceed the saturated hydraulic conductivity of the surficial soil through which it must travel; otherwise ponding would occur.

- Potentiometric lines on streams that are gaining water should point upstream, whereas the lines should point downstream along losing streams.

- Ephemeral streams generally should not be modeled as constant head boundaries. Transient boundaries should be clearly identified.

- Streams are frequently modeled as ground-water divides, that is, all ground-water flowing towards the stream is assumed to be captured by the stream. The modeler should justify this assumption, as not all streams fully penetrate the aquifer.

- In the natural system, boundaries may shift with time, and the effect that these positional changes may have on the results of modeling should be considered.

- Surface-water/ground-water interactions should be discussed.

- The transient nature of boundaries should be described.

- Recharge and evapotranspiration are difficult to determine, and therefore, recharge as a flux boundary is often used as a calibration parameter. The method for determining recharge should be presented.

- Interpretation and extrapolation methods (e.g., Kriging) should be described.

- Boundaries between two types of porous media should coincide with grid and layer boundaries.

Calibration

- Decision process flow diagrams or other means should show the approach that was taken to calibrate the model.

- The calibration process should be described in detail, including any assumptions and limitations.

- The objectives of calibrating heads and flows should be presented.

- The sources and magnitudes of errors should be described, particularly the potential effects on the predictive simulations which will be performed later.

- Modifications to the parameter values, boundary conditions, and imposed hydraulic stresses should be discussed in detail, particularly focusing on the response of the modeled system to the altered values and the rationale for the changes.

- The rationale for the convergence criterion for the heads and concentrations should be presented, in addition to a discussion of the overall mass balance results.

- Problems that arose due to failure of the code to converge or numerical instabilities should be described.

- The calibrated parameter values should be compared with the initial range of these parameters. Particular emphasis should be placed on parameters that fall outside their originally estimated range.

- If both steady-state and transient calibrations are performed, their similarities and differences within the results should be discussed. The rationale and selection of time steps for the transient calibration should be discussed.

- The mass-balance results should be discussed.

- The calibrated model should be a good match with the conceptual model, such as flow directions and parameter values.

- The results should meet the calibration targets.

- The water balance error should be less than 1%.

- The calibrated parameters, especially hydraulic conductivity, should not appear patch worked. Unless there is evidence indicating that hydraulic conductivity values change substantially from one grid block to the next, it should be assumed that large percentages of the modeled area are relatively homogeneous.

- Areal recharge should be uniform unless there is sufficient justification to vary the recharge rates locally.

- Well logs and aquifer stress test data should be reviewed to ensure that the hydraulic conductivities assigned to that area are compatible.

- The volume of water entering or exiting local streams, lakes, or rivers should be consistent with the field data.

- It should be kept in mind that head and concentration values computed at a node are representative of an area rather than a point. Model calibration over a short period of time where there is a large variation in hydraulic heads, such as during a pumping test, should be avoided.

- Vertical gradients within an aquifer in which the well is not fully penetrating should be considered when the model is calibrated.

- A list and a figure indicating the final calibrated values for parameters and boundary conditions should be included.

- The match to the calibration targets should be shown in figures as well as in tables. Sections within the model should be outlined and discussed according to their "goodness of fit" to the calibration targets.

- Particle tracking should be shown in planar and cross-sectional views.

A.7.1.g. SENSITIVITY/UNCERTAINTY ANALYSIS

Many of the modeling scenarios will involve parameters that can vary over a considerable range and field measurements of many parameters are lacking. For this reason, the sensitivity of model predictions to key model parameters should be documented. Documentation should include the following:

- The approach undertaken for the sensitivity analysis should be detailed.

- The rationale for selecting parameters for the sensitivity analysis and for determining whether there were sufficient simulations investigating single or multiple parameters should be presented.

- The sensitivity of model calibration quality and model predictions to variations in parameter values, including grid spacing, time steps, and boundary conditions, should be discussed, emphasizing parameters in which there is a large degree of uncertainty and the results are very sensitive.

- The relevance of the overall uncertainty and sensitivity with respect to the objectives of the predictive simulations should be discussed.

- The results of the sensitivity analysis should be displayed in a graph as well as in narrative form.

- A range tested for selected parameters and how they were chosen.

- How sensitivity coefficients or other measures of model sensitivity were computed.

A8 SPECIAL TRAINING REQUIREMENTS/CERTIFICATION

EPA, States, and the regulated community employ ground-water models for a variety of purposes including evaluations of corrective action options and remedial studies, risk assessment, performing wellhead assessments, evaluating possible leachate migration from solid non-hazardous waste landfills, mine closure planning and acid mine drainage problems, understanding contaminant fate and transport at hazardous waste sites, supporting State risk reduction programs, evaluating natural attenuation, mass balance geochemical modeling, and uses of models by permit applicants. Ground-water modeling may be a formidable task due to the complexity of the underlying sciences and because of the type and level of specialized expertise needed to carry out the array of modeling related tasks. While no formal Federal licenses/certifications are necessary, the project manager will have credentials commensurate with typical state requirements for industry experts (i.e., state P.G. license). Other individuals involved with this project, including potential reviewers, have education and experience in geology and hydrogeology, hydrology, engineering, mathematics, chemistry, and applied ground-water modeling. If, during the course of this modeling project additional skills, training, and continuing education are needed, the Agency will seek to fulfill these additional requirements as appropriate.

A9 DOCUMENTATION AND RECORDS

Documentation of the modeling process is crucial for assuring the defensibility of the modeling application and for providing enough information so that a thorough review may be conducted. The EPA Geologist/Modeler will maintain and archive all modeling files (hard copy and electronic) in accordance with Agency records management requirements. Most files will be kept electronically. In general, modeling files are expected to be categorized as follows:

- Files for Conceptual Model
- Files for Water Level Data
- Files Related to Contaminant Concentrations
- Base maps and aerial photos
- Data sets for initial conditions; calibration data sets
- Files for individual model runs
- Report Files
- Model Review Files
- QAAP Files

For electronic files, the size of any particular file and ability to access the information during model development will determine the optimum electronic file storage device and backup file location (e.g., computer hard drive, EPA network drive, etc.). Individual model run files (e.g., Modflow and MT3D files) will be stored on the EPA network drive, 'B0606gdaec005\users'(R), in a folder labeled "KAFB Model Runs". Supporting files will be under folders labeled "Kirtland Air Force Base BFF Fuel Spill Groundwater Modeling Project" (R or H drive), and/or simply listed as "Kirtland". Backup copies of model versions and runs will be located on the EPA Geologist/Modeler's computer (computer #B20185) with the same file names.

GROUP B MEASUREMENT AND DATA ACQUISITION

The sections below address Group B, Sections B7, B9, and B10, which are referenced by "*EPA Guidance for Quality Assurance Project Plans for Modeling"* (EPA 2002) as being especially relevant for modeling.

B7 MODEL CALIBRATION

The purpose for calibrating this model is to produce simulated water levels, gradients, and contaminant transport results over the main area of interest that are generally consistent with field measurements. Calibration of flow and contaminant boundaries will be attempted to the degree sufficient data are available. Model calibration will be illustrated and quantified utilizing software functions integral to the data processor, producing statistically derived graphs and plots, and by making adjustments through model iterations to minimize differences between simulated and observed values. Additional model checks will be made from making hand calculations to further examine and compare results for well drawdown, area of influence of pumping wells, and groundwater velocity as necessary. Data to be used for calibration will be identified in KAFB reports and also other published and unpublished reports including reports on regional and local water level data, and any available data from municipal and other industry sources. Any deficiencies identified in calibration will be resolved to the extent possible by adjusting model input parameters, initial conditions, and boundary conditions so that the model simulates the aquifer system and contaminant fate and transport to a desired level of accuracy and reliability. The degree of success in calibration will be presented in the final modeling report.

Following a MODFLOW run, and similarly for contaminant concentrations from MT3D, head equipotential contours and contaminant concentrations will be displayed along with a calibration plots/targets dialog box. Within the calibration plots dialog box the modeler can select individual sets of monitoring well data and the type of calibration statistic/graph to review. Several calibration statistics may be produced including the Calibration Residual, Residual Mean, Absolute Residual Mean, Standard Error of the Estimate, Root Mean Squared, and the Normalized Root Mean Squared. The following equations are summarized from Schlumberger Water Services Visual Modflow User's Manual (v 4.3).

Calibration Residual (Eq. 1)

The Calibration Residual (Ri) is the difference between the calculated results (Xcalc) and the observed results (Xobs).

$$Ri = Xcalc - Xobs$$

<u>Residual Mean (Eq. 2)</u>

The Residual Mean ($\overline{R}$) is a measure of the average residual value defined by:

$$\boldsymbol{\overline{R} = \frac{1}{n}\sum_{i=1}^{n} Ri}$$

<u>Absolute Residual Mean (Eq. 3)</u>

The Absolute Residual Mean $|\overline{R}|$ is similar to the Residual Mean. It measures the average magnitude of the Residuals therefore provides a better indication of calibration than the Residual Mean.

$$\boldsymbol{|\overline{R}| = \frac{1}{n}\sum_{i=1}^{n} |Ri|}$$

<u>Standard Error of the Estimate (Eq. 4)</u>

The Standard Error of the Estimate (SEE) indicates the variability of the residual around the expected residual value:

$$\boldsymbol{SEE = \sqrt{\frac{\frac{1}{n-1}\sum_{i=1}^{n}(Ri - \overline{R})^2}{n}}}$$

<u>Root Mean Squared (Eq. 5)</u>

The Root Mean Squared (RMS) is given by the following equation:

$$\boldsymbol{RMS = \sqrt{\frac{1}{n}\sum_{i=1}^{n} Ri^2}}$$

Normalized Root Mean Squared (Eq. 6)

The Normalized Root Mean Squared is the RMS divided by the maximum difference in observed head values:

$$\boldsymbol{Normalized\ RMS} = \frac{\boldsymbol{RMS}}{(\boldsymbol{Xobs})\,\mathbf{max} - (\boldsymbol{Xobs})\boldsymbol{min}}$$

The Normalized RMS is expressed as a percentage and is more representative of a fit of measure than the standard RMS, because it accounts for the scale of the potential range of data values.

The residual distribution graph displays the residual distribution for selected observation wells. This graph depicts the population, frequency, or relative frequency of observations for specified intervals of normalized calibration residual values. The head versus time graph displays the head versus time for selected observation wells. This graph presents time series plot of observed and calculated heads for each observation point selected. The statistics versus time graph include the normalized RMS versus time, residuals versus time, normalized residuals versus time, and error versus time. In terms of calibration for contaminant fate and transport, graphs are also available for calculated versus observed concentrations and concentration versus time.

Well Drawdown (Eq. 7)

Since there are pumping wells within the project area, comparisons will be made between simulated drawdown from Modflow and calculated drawdown from the nonequilibrium equation (Theis equation) at selected wells. The purpose of the comparison is to provide a quality check on computer output. Well drawdown will be calculated using the equations below.

$$\boldsymbol{ho - h} = \frac{\boldsymbol{Q}}{\boldsymbol{4\pi T}} \int_{\boldsymbol{u}}^{\infty} \frac{\boldsymbol{e^{-a}}}{\boldsymbol{a}}\, \boldsymbol{da}$$

<u>Well Function (Eq. 8)</u>

Then, substituting the well function W(u), the equation becomes:

$$\boldsymbol{ho - h = \frac{Q}{4\pi T} W(u)} \qquad\qquad Where:\ u = \frac{r^2 S}{4Tt}$$

r = radial distance from pumping well
S = aquifer storativity
T = aquifer transmissivity
t = time since pumping began

The well function term W(u) will be obtained from Fetter (2001), Appendix 1.

B9 NON-DIRECT MEASUREMENTS

The model will mainly rely on existing non-direct measurement data available in reports produced by government agencies. Some new data may also be included, from routine groundwater monitoring reports (i.e., quarterly/semi-annual reports) depending on the time-frames established in the model for model calibration and boundary conditions.

Data from existing non-measurement sources will include published and unpublished information obtained from NMED, KAFB, EPA, USGS, ABCWUA, the New Mexico Bureau of Geology and Mineral Resources, and other credible organizations. Generally, only information obtained from peer reviewed, published, and authoritative scientific information sources will be utilized in the model in order to ensure an acceptable level of data quality. Comparisons of data from different time periods will be made to ensure that model data are representative, and any data anomalies are identified and considered.

EPA will utilize the services of the EPA Region 6 Library to conduct a thorough literature search. The EPA Library (and Library Network), established in 1971, includes libraries in the Agency's Washington, D.C. Headquarters, all 10 Regional EPA Offices, and Agency laboratories located throughout the United States. The combined Library network collection contains a wide range of general information on environmental protection and management; the basic sciences such as geology, biology and chemistry; the applied sciences such as engineering and toxicology; and extensive coverage of topics featured in legislative mandates such as hazardous waste, drinking water, pollution prevention, and toxic substances. The Region 6 Library, at the request of the project manager, will search for literature e for specified subjects related to the geology and hydrogeology of the Albuquerque area and specifically for information related to the Sante Fe aquifer at the project area.

Certain types of site-specific information are more readily obtained from KAFB and NMED files than from general literature. KAFB maintains a set of technical documents at http://www.kirtland.af.mil/environment.asp, and NMED posts technical information on the department's FTP directory at ftp://ftp.nmenv.state.nm.us/hwbdocs/HWB/KAFB/Bulk_Fuels_Facility_Spill/. Documents from these websites will be accessed for important data and verified/discussed with knowledgeable NMED or KAFB staff to ensure accuracy. This will include water levels, site specific geologic conditions, well construction information, contaminant concentration data, and similar information.

The data processor is capable of importing information on existing water wells for both pumping wells and groundwater monitoring wells. The most important wells to this project are: (i) those in the model domain which influence water and contamination movement in the Sante Fe aquifer, (ii) those that will be used for matching simulated and observed hydraulic heads, and (iii) those that can be used to calibrate model boundaries. For pumping wells, data to be imported includes well depth, pumping schedule, screened interval, pumping rates, and location coordinates; and for monitoring wells, data includes depth, screened interval, water level measurements, and contaminant concentrations.

B10 DATA MANAGEMENT AND HARDWARE/SOFTWARE CONFIGURATION

This section introduces the computer modeling programs MODFLOW, MODPATH, and MT3D. The selected data processor is Visual Modflow. Certain sections of the following discussion about MODFLOW were taken from the U.S. Geological Survey public domain website www.water.usgs.gov.

MODFLOW is a Modular Three-Dimensional Finite-Difference Ground-Water Flow Model that was developed by the U.S. Geological Survey (McDonald and Harbaugh, 1988; Harbaugh and McDonald, 1996) during the early 1980s. MODFLOW is the world-wide standard ground-water flow modeling program because of its ability to simulate a wide variety of ground-water systems, its extensive publically available documentation, and its rigorous USGS peer review. MODFLOW does not contain a mass transport component by itself. When properly utilized, MODFLOW is the standard model used by regulatory agencies, universities, consultants, and industry for ground-water investigations, development of remedial designs, and is accepted as suitably reliable for use in legal proceedings.

MODFLOW is designed to simulate aquifer systems in which (1) saturated-flow conditions exist, (2) Darcy's Law applies, (3) the density of ground-water is constant, and (4) the principal directions of horizontal hydraulic conductivity or transmissivity do not vary within the system. These conditions are met for many aquifer systems for which there is an interest in analysis of ground-water flow and contaminant movement. For these systems, MODFLOW can simulate a wide variety of hydrologic features and processes. Steady-state and transient flow can be simulated in unconfined aquifers, confined aquifers, and confining units. A variety of features and processes such as rivers, streams, drains, springs, reservoirs, wells, evapotranspiration, and recharge from precipitation and irrigation also can be simulated. At least four different solution methods have been implemented for solving the finite-difference equations that MODFLOW constructs. The availability of different solution approaches allows model users to select the most efficient method for their problem. MODFLOW simulates ground-water flow in aquifer systems using the finite-difference method. In this method, an aquifer system is divided into rectangular blocks by a grid. The grid of blocks is organized by rows, columns, and layers, and each block is commonly called a "cell." For each cell within the volume of the aquifer system, the user must specify aquifer properties. Also, the user specifies information relating to wells, rivers, and other inflow and outflow features for cells corresponding to the location of the features. For example, if the interaction between a river and an aquifer system is simulated, then for each cell traversed by the river, input information includes layer, row, and column indices; river stage; and hydraulic properties of the river bed. MODFLOW uses the input to construct and solve equations of ground-water flow in the aquifer system. The solution consists of head (ground-water level) at every cell in the aquifer system (except for cells where head was specified as known in the input data sets) at intervals called "time steps." The head can be printed and (or) saved on a computer storage device for any time step. Hydrologists commonly use water levels from a model layer to construct contour maps for comparison with similar maps drawn from field data. They also compare computed water levels at individual cells with measured water levels from wells at corresponding locations to determine mode error. The process of adjusting the model input values to reduce the model error is referred to as model calibration. In addition to water levels, MODFLOW prints a water budget for the entire aquifer system. The budget lists inflow to and outflow from the aquifer system for all hydrologic features that add or remove water. Other program output consists of flow rates for each model cell. MODFLOW can write the flow rates onto a computer storage device for any hydrologic feature in a simulation. These cell-by-cell flow rates commonly are read by post-processing programs for detailed analysis of the simulated ground-water system.

In addition to MODFLOW, a program called MODPATH (Pollock, 1989) will be utilized for particle tracking. MODPATH is a particle tracking post-processing package designed to work with MODFLOW. Output from steady-state or transient MODFLOW simulations is used in MODPATH to compute paths for imaginary “particles” of water moving through the simulated ground-water system. MODPATH also keeps track of the time of travel for particles moving through the system. By carefully determining the starting position of particles, it is possible to use MODPATH to perform a wide range of analyses, such as delineating capture and recharge areas or drawing flow nets.

The modeling code dealing with contaminant fate and transport is expected to be Mass Transport in Three Dimensions (MT3D) or Reactive Transport in Three Dimensions (RT3D). The selection of code will depend on the conceptual model and on the degree to which any chemical reactions need to be simulated. MT3D is a modular three-dimensional transport program for simulation of advection, dispersion, and chemical reactions of contaminants in ground-water. MT3D is intended for use with MODFLOW or any other finite-difference flow model, and is based on the assumption that changes in the concentration field will not substantially affect the flow field. RT3D is based on MT3D, is for simulating reactive multi species transport in three-dimensional ground-water aquifers.

To assist with running MODFLOW, MODPATH, and MT3D or RT3D, an additional data processing program will be used called Visual Modflow. Visual Modflow is a proprietary modeling program produced by Schlumberger Water Services Inc., and is designed to facilitate model development, data input, calibration, and the visualization of model output. Visual Modflow has three main modules: the Input Module, Run Module, and Output Module. The Input Module allows the user to graphically assign all of the necessary input parameters for building a three-dimensional ground-water flow model. The input menus represent the basic model building blocks for assembling a data set for MODFLOW, MODPATH, and ZoneBudget (a water balance program). The menus are displayed in logical order and guide the modeler through steps necessary to design a ground-water flow model. In the Run Module, the user specifies parameters and options which are run-specific. These include selecting initial head estimates, setting solver parameters, activating the re-wetting package, specifying output control, etc. Each of these menu selections has default settings which may be changed by the modeler as warranted. The Output Module allows the user to display modeling and calibration results, and allow the user to select, customize, and overlay various display options for presenting modeling results. Numerical model data management is an integral component of Visual Modflow. Visual Modflow stores all data as a set of data files. Input files are ASCII files, however some output files are binary. If any formatting mistakes are in the input file, Visual Modflow will not process the data. The Visual Modflow User's Manual lists all data files and describes their formats, and the reader is referred to the manual for detailed information. The file extension .vmf contains the basic project file.

GROUP C ASSESSMENT AND OVERSIGHT
C1 ASSESSMENT AND RESPONSE ACTION

Element C1 describes the different types of assessments and model performance evaluations to be conducted during the model development and application process. These assessment and evaluation activities will ensure that the quality objectives and criteria for model input/outputs in Section A71 Model Development and Quality Review Criteria are being fully achieved. These activities essentially formulate checks and balances using internal and external assessments to ensure the highest data quality given the project scope and magnitude.

Internal and External Reviews

Technical assistance will be requested from internal and external organizations during model development and application. Internal assistance will be requested from the EPA Office of Research and Development, R.S. Kerr Environmental Research Laboratory in Ada, Oklahoma. This will involve meeting with hydrogeologists and modelers to discuss critical model design features (such as boundary conditions) to ensure that model setup is appropriate. External assistance will be requested from Schlumberger Inc, the data processor software vendor, to assist with model calibration and ensure that software is being applied properly. The response action to these reviews will be to consider any suggested modifications and improvements and implement changes which are consistent with quality objectives and model goals.

EPA will also seek input from NMED regarding the site-specific nature of the subsurface and the known extent of contamination near the Bulk Fuels Facility. Other routine assessments will be performed during model development and application and will generally be conducted informally as part of the day-to-day work towards developing a reliable model. These are described below.

Objectives and Data Requirements

An initial data review will be conducted to determine the extent of available data to support a groundwater model. This will include geologic and hydrogeologic data, ground-water level data, boundary data, pumping rates and schedules of recovery well(s), recharge data within the model area, contaminant concentration/plume chemistry information, and other related information. The assessment will determine whether the data are sufficient to support the planned ground-water model to meet project goals and objectives. The assessment should evaluate data uncertainty, limitations, weaknesses, and usefulness. After complete review of available data, the project will either move forward to building the Conceptual Model, or a recommendation will be made for collecting additional data needed to ensure that a model can be developed that meets the project objectives. Any recommendations for significant additional data needs will be provided to the Chief of the Corrective Action and Waste Minimization Section as indicated on the project organizational chart contained in Section A4, and/or discussed with NMED.

Review Considerations for Conceptual Model Development

If the initial data assessment described above concludes that available input data are acceptable and adequate for modeling purposes, the next phase would be developing the Conceptual Model. While building the conceptual model, the assessment process will evaluate:

- Whether the hydrogeologic system can be adequately described with available data to meet project objectives,

- Whether water budget analysis is projected to be adequate to describe inflow and outflow, system boundaries, and flow between layers, and

- Uncertainties in the conceptual model and their possible effect on model output.

Once the Conceptual Model is complete the assessment will evaluate if the Conceptual Model meets the criteria listed in Section A7.1.d. The response would be to determine whether a numerical model based on the Conceptual Model will meet the project objectives, or whether a recommendation will be made for collecting additional data needed for an adequate Conceptual Model. If the Conceptual Model is satisfactory and meets the criteria listed in Section A.7.1.d, the project will move forward towards building the numerical model. If the Conceptual Model does not meet the criteria listed in Section A7.1.d., the Chief of the EPA Corrective Action and Waste Minimization Section and the Region 6 Quality Assurance Manager shall be notified.

Code Selection

The selected codes MODFLOW, MODPATH, and MT3D/RT3D are public domain, industry standards and have been used extensively for many years. Therefore, a rigorous assessment of the selected codes is not required. However, the assessment process should evaluate whether the selected models, with their underlying assumptions and limitations, are capable of meeting the project objectives outlined in Section A5.

Model Construction, Simulations, and Calibrations

Once construction of the numerical model is underway, several assessments will be performed throughout the model development process to ensure that model development and calibration criteria established in A.7.1.f are being satisfied. The model may require calibration to both steady-state and transient conditions. An initial steady-state model assuming average conditions may be calibrated to estimate input parameter distribution. A transient calibration may follow to improve parameter estimation such as aquifer hydraulic conductivity and boundary conductance. If preliminary model results do not satisfy the target calibration criteria, all possible errors and accuracy of input data, model framework, and field observations will be thoroughly investigated. If adjustments to calibration criteria or model objectives are needed, they will be fully documented, and revisions to this combined QAPP and Work Plan will be issued through the formal QA process. Once a satisfactory calibration is achieved the model may be validated depending on project schedule and end user need. If validation is conducted, validation will be accomplished by utilizing observed water levels and contamination data not used in the calibration data set. Because of the time required to collect validation data outside of the calibration data set, EPA may issue a final project report prior to validation taking place.

Sensitivity Analysis

Sensitivity of model output to key model input parameters over their expected range of variability will be assessed in the final stage of the numerical modeling process. In particular, sensitivity to aquifer properties, boundary condition values, and pumping rates will be evaluated. The sensitivity analysis may evaluate how uncertainty in model output may be reduced in a cost-effective manner during future data gathering efforts. Sensitivity evaluations will consist of comparison of model results with observed historical data, and general evaluations to ensure reasonable model behavior for output lacking historical data. The assessment will analyze output data and determine possible anomalies or departures from assumptions made during the planning phase.

Uncertainties

A discussion of modeling uncertainties will be included to describe the main uncertainties encountered and how they were addressed. Uncertainties require making assumptions during model construction and the setup of individual model runs. In general, uncertainties will be addressed by considering all available site-specific and/or regional data, as appropriate, and by using such information with professional judgment and reviews to bridge data gaps and produce reasonable model output.

C2 REPORTING TO MANAGEMENT

A final QA report will be provided to Management and the Division QA Officer at the completion of the project. Periodic reporting to Management will also occur during normal staff/Management meetings and through any special requested status reports. The modeling project manager will prepare the final QA report.

GROUP D DATA VALIDATION AND USABILITY

D1 DEPARTURES FROM VALIDATION CRITERIA

Model reviews, assessments, and validation are discussed in Section C1. Section C1 also addresses how departures from calibration and validation will be addressed and the necessary response actions. Model validation may take place depending on the need per discussions with NMED.

D2 VALIDATION METHODS

Model validation requires a commitment to gather and use data which is separate from data used for model construction. For any such data collected, it will be compared with model output to provide validation to the model results.

D3 RECONCILIATION WITH USER REQUIREMENTS

Upon completion of numerical modeling incorporating assessment procedures outlined in Section C1, a draft report will be prepared for review. The document will provide a detailed description of groundwater flow and contaminant fate and transport in the Sante Fe aquifer near the Bulk Fuels Facility and nearby water supply wells. The report will describe data review, calibration, sensitivities, and uncertainties as presented in Section C to confirm the steps of modeling process were followed correctly. The report will address all pertinent A5, A7, and group B elements and present results that meet the project objectives, and will describe and justify departures from any criteria set in this QA plan. The report will discuss if outputs are the right type, quality, and quantity needed to meet project objectives and will describe limitations of the output data that may impact usability. During preparation of the final report, the following table will be used as a checklist to ensure major steps in the modeling evaluation procedure have been completed. Contents of the final report will be reflective of the Table of Contents contained in A6.

Table 2: Model Evaluation Appraisal

MODELING AND EVALUATION CRITERIA	APPRAISAL		
	Yes	No	Comments
OBJECTIVES AND DATA REQUIREMENTS			
Are the purpose and scope outlined?			
Are the objectives consistent with decision-making needs?			
Are the objectives satisfactory?			
Are a site description and waste disposal history provided?			
Are the data requirements for the proposed modeling outlined?			
Are the sources of data adequately presented?			
Are data uncertainties discussed?			
Is the probable sensitivity of the future modeling results presented for the data?			
Are the potential data limitations and weaknesses provided?			
Are the plans to resolve data limitations discussed?			
Is the physical framework discussed in detail? Both regional and local?			
Is the hydrogeologic framework described in detail? Both regional and local?			
Are the hydraulic boundaries described in detail?			
Is the conceptual model consistent with the field data?			
Are the uncertainties inherent in the conceptual model discussed?			
Are the simplifying assumptions outlined?			
Are the assumptions justified?			
Are the following figures and/or tables[1] *included:*			
· Map showing location of study area.			
· Geologic map and cross sections indicating the areal			

In some instances tabular representation of the data may be appropriate.

MODELING AND EVALUATION CRITERIA	APPRAISAL Yes	No	Comments
and vertical extent of the system.			
· Topographic map with the surface water bodies.			
· Contour maps showing the tops and/or bottoms of the aquifers and confining units.			
· Isopach maps of hydrostratigraphic units.			
· Maps showing extent and thicknesses of stream and lake sediments.			
· Maps indicating discrete features (e.g., faults), if present.			
· Maps and cross sections showing the unsaturated zone properties (e.g., thickness, K_{sat}).			
· Potentiometric surface maps of aquifer(s) and hydraulic boundaries.			
· Maps and cross sections showing storage properties of the aquifers and confining units.[1]			
· Maps and cross sections showing hydraulic conductivity of the aquifers, confining units, and stream and lake sediments (if applicable).			
· Maps and hydrographs of water-budget information.			
SCOPING ANALYSIS			
Are scoping analyses performed?			
Do scoping results lead to proposed modeling approach?			
SITE CHARACTERIZATION MODELING			
Code Selection			
Is the rationale for the selection clearly presented for proposed code(s)?			
Are the general features of the code(s) presented?			
Are the assumptions and limitations of the code(s) presented and compared to the conceptual model?			

MODELING AND EVALUATION CRITERIA	APPRAISAL		
	Yes	No	Comments
Is the basis for regulatory acceptance presented?			
Does the code have a history of use?			
Is the code well documented?			
Is the code adequately tested?			
Are the hardware requirements compatible with those available?			
Model Construction			
Layering and Gridding:			
Is the domain of the grid large enough so that the boundaries will not interfere with the results?			
Do the nodes fall near pumping centers on existing and potential future wells and along the boundaries?			
Is the grid oriented along the principal axes of hydraulic conductivity?			
Is the grid discretized at the scale appropriate for the problem?			
Are areas of sharp contrasts (e.g., hydraulic conductivity, concentration, gradient) more finely discretized?			
Do adjacent elements vary in size by a distance less than a factor of 1.5?			
Are strong vertical gradients within a single aquifer accommodated by multiple planes or layers of nodes?			
If matrix diffusion is important, are the confining units adequately discretized in the relevant regions of the model?			
Is the grid more finely spaced along the longitudinal direction of simulated contaminant plumes?			
Is the aspect ratio less than 100:1?			
Are the following figures included:			
· Grid presented as an overlay of a map of the area to be modeled.			
· A vertical cross section(s) which displays the vertical layering of the model grid.			
Boundary and Initial Conditions			

MODELING AND EVALUATION CRITERIA	APPRAISAL		
	Yes	No	Comments
Is justification provided for the selection of all boundary and initial conditions?			
Are model boundaries consistent with natural hydrologic features?			
Are the boundary and initial conditions consistent with the conceptual model?			
Are the uncertainties associated with the boundaries and initial conditions addressed?			
Are the boundaries far enough away from any pumping/injection centered to prevent "boundary effects"?			
Are transient boundaries discussed?			
Is the rationale given for simplifying the boundaries from the conceptual model discussed?			
Are the values for the assigned boundaries presented?			
Model Parameterization			
Are data input requirements fully described?			
Is the discussion of the data well founded with respect to Objectives and Data Review Section?			
Are the interpretation and extrapolation methods (e.g., Kriging) adequately presented?			
Do the figures and tables completely describe the data input with respect to discrete components of the model?			
Are the model parameters within the range of reported or measured values?			
MODEL CALIBRATION			
Has calibration been attempted?			
Is the rationale for model calibration approach presented?			
Are the calibration procedures described in detail?			
Are the calibration criteria presented?			
Does the calibration satisfactorily meet specified criteria?			
Is the rationale presented for selecting convergence criteria?			

MODELING AND EVALUATION CRITERIA	APPRAISAL		
	Yes	No	Comments
Are code convergences and numerical instabilities discussed?			
Do the calibrated parameters fall within their expected ranges?			
Are discrepancies explained?			
Has the calibration been tested against actual field data?			
Are the differences between steady-state and transient calibrations presented?			
Could other sets or parameters have calibrated the code just as well? Is this discussed?			
Are areal and cross-sectional representations of the final calibrated results included for both hydraulic heads ?			
Does calibration of the model take into account the inconsistency between point measurements at wells and areal averages of model output?			
Is the match between the calibration targets and final parameters shown diagrammatically?			
Were calibrating errors presented quantitatively through the use of descriptive statistics?			
If particle-tracking was performed, are these results shown?			
Is the calibrated model consistent with the conceptual model?			
Are any changes to the conceptual model discussed and justified?			
Is non-uniform areal recharge applied? Is this approach justified?			
Does the calibration properly account for vertical gradients?			
Is the calibrated hydraulic conductivity field consistent with the geologic logs and aquifer stress tests?			
Are the convergence criteria appropriate?			
Was a mass balance performed?			
Is the water-balance error less than 1%?			
Are the mass balance results for the calibrated model discussed?			
Is the model's water balance consistent with known flows of rivers and levels of lakes?			

MODELING AND EVALUATION CRITERIA	APPRAISAL		
	Yes	No	Comments
SENSITIVITY ANALYSES			
Was a sensitivity analysis performed?			
Is the approach to the sensitivity analysis detailed?			
Were all input parameters selected for investigation? If not, was rationale presented for excluding parameters?			
Was a sensitivity analysis performed on the boundary conditions?			
Are the ranges of parameters appropriate?			
Were sufficient simulations performed? Was justification provided?			
Was the relevance of the sensitivity analysis results to the overall project objectives discussed?			
Are the results presented so that they are easy to interpret?			
Were sensitivity analyses performed for both the calibration and the predictive simulations?			

REFERENCES

American Society for Testing and Materials, 2002, *Annual Book of Standards Volume 4.08.* Philadelphia, Pennsylvania.

Harbaugh, A.W. and McDonald, M.G., 1996, *User's documentation for MODFLOW-96, an update to the U.S. Geological Survey modular finite-difference ground-water flow model*, U.S. Geological Survey, Washington, D.C.

McDonald, M.G. and Harbaugh A.W., 1988*, A modular three-dimensional finite-difference groundwater flow model*: U.S. Geological Survey, Washington, D.C.

Pollock, D. W., 1994, *User's guide for MODPATH/MODPATH-plot, version 3: A particle tracking post processing package for MODFLOW, U.S. Geological Survey Finite-Difference Ground-water Flow Model,*U.S. Geological Survey, Washington, D.C.

U.S. Army Corps of Engineers, 1999, *Engineering and Design - Groundwater Hydrology,* Manual No. 1110-2-1421, Washington, D.C.

U.S. EPA, 1996, *Documenting Ground-Water Modeling at Sites Contaminated with Radioactive Substances,* EPA 540-R-96-003, Office of Air and Radiation, Washington, DC.

U.S. EPA, 1998a., *EPA Guidance for Quality Assurance Project Plans: EPA QA/G-5,* EPA/600/R-98/018, Quality Assurance Management Staff, Washington, D.C.

U.S. EPA, 1999a, *Data Quality Objectives Process for Hazardous Waste Site Investigations*, EPA QA/G-4HW Peer Review Draft.

U.S. EPA, 1999b, *Guidance for Data Quality Objectives Process, Final,* EPA QA/G-4 Peer Review Draft.

U.S. EPA, 2000*, EPA Quality Manual for Environmental Programs, Office of Environmental Information, Quality Staff, Washington, D.C.*

U.S. EPA, 2000a, *Policy and Program Requirements for the Mandatory Agency-wide Quality System,* EPA Order 5360.1 A2, Washington D.C.

U.S. EPA, 2000b*, EPA Quality Manual for Environmental Programs* (Order 5360 A1), Washington, D.C.

U.S. EPA, 2001, *EPA Requirements for Quality Assurance Project Plans for Environmental Data Operations QA/R-5,* EPA/240/B-01/003, Washington, D.C.

U.S. EPA, 2002*, Guidance for Quality Assurance Project Plans for Modeling, QA/G-5M,* EPA/240/R-02/007, Office of Environmental Information, Quality Staff, Washington, D.C.